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Some graft transformations and its applications on the distance spectral radius of a graph

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ABSTRACT

Let $D(G) = (d_{i,j})_{n\times n}$ denote the distance matrix of a connected graph G with order n, where d_{ij} is equal to the distance between v_i and v_j in G. The largest eigenvalue of $D(G)$ is called the distance spectral radius of graph G, denoted by $\varrho(G)$. In this paper, some graft transformations that decrease or increase $\varrho(G)$ are given. With them, for the graphs with both order n and k pendant vertices, the extremal graphs with the minimum distance spectral radius are completely characterized; the extremal graph with the maximum distance spectral radius is shown to be a dumbbell graph (obtained by attaching some pendant edges to each pendant vertex of a path respectively) when $2 \le k \le n-2$; for $k = 1, 2, 3, n-1$, the extremal graphs with the maximum distance spectral radius are completely characterized.

1. Introduction

The distance matrix of a graph, while not as common as the more familiar adjacency matrix, has nevertheless come up in several different areas, including communication network design [1], graph embedding theory [2–4], molecular stability [5,6] and network flow algorithms [7,8]. So it is very interesting to study the spectra of these matrices.

Throughout this article, all graphs considered are simple, connected and undirected. Let $G = G[V(G), E(G)]$ be a graph with vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ is the order and $|E(G)| = m$ is the size of G. Let $N_G(v)$ denote the set of the vertices adjacent to v in G. The degree of v in G, denoted by $deg(v)$, is equal to $|N_G(v)|$. A vertex is called a pendant vertex if its degree is 1. We denote by P_n, K_n, S_n a path, a complete graph, a star with order n, respectively. In a graph G, the length of a shortest path from v_i to v_j is called the distance between v_i and v_j, denoted by $d(v_i, v_j)$ or $d_G(v_i, v_j)$. $d(G) = \max d(v_i, v_j) \mid v_i, v_j \in V(G)$ is called the *diameter* of graph G. Let $P_{i,j}$ denote a shortest path from vertex v_i and v_j. If the length of the path $P_{i,j}$ is equal to $d(G)$, then $P_{i,j}$ is called a *diameter-path*, and v_i, v_j are called the end vertices of $P_{i,j}$. For $S \subseteq V(G)$, let $G[S]$ denote the subgraph induced by S. For a vertex set $\{v_1, v_2, \dots, v_k\}$, we sometimes abbreviate $G[\{v_1, v_2, \dots, v_k\}]$ as $G[v_1, v_2, \dots, v_k]$. The dumbbell graph $D(n; s, p)$ consists of a path P_{n-s-p}, s pendant edges attaching to a pendant vertex of P_{n-s-p} and p pendant edges attaching to the other pendant vertex of P_{n-s-p} ($s \ge 0, p \ge 0, s+p \le n-2$). Denote by $\mathscr{D}(n, k; s, p) = \{D(n; s, p) \mid s+p = k\}$.

Let $D(G) = (d_{i,j})_{n\times n}$ denote the distance matrix of a connected graph G with order n, where $d_{ij} = d_G(v_i, v_j)$. The distance characteristic polynomial of G, denoted by $P(D(G))$ (or $P(D(G), \lambda)$), is defined as $\det(\lambda I - D(G))$, where I is the

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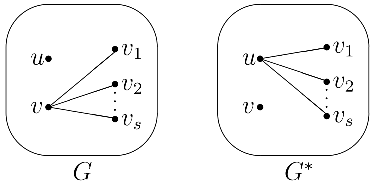

Fig. 1.1. Graft transformation.

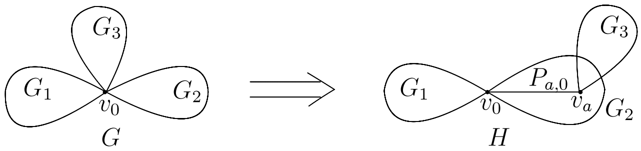

Fig. 2.1. G, H.

identity matrix. The largest eigenvalue of $P(D(G))$ is called the distance spectral radius of G, denoted by $\varrho(G)$. By the Perron–Frobenius theorem [9], for a connected graph G, we know that there exists a unit positive vector corresponding to $\varrho(G)$ which is called *Perron eigenvector*. The pendant number of a graph G, denoted by $\mathcal{K}(G)$, is the number of pendant vertices. Let $\mathscr{G}(n; k) = \{G \mid G$ be a graph with order n, $\mathcal{K}(G) = k\}$, $\mathscr{T}(n; k) = \{T \mid T$ be a tree with order n and $\mathcal{K}(T) = k\}$, $\varrho_{max}(\mathscr{G}; n, k) = \max\{\varrho(G) \mid G \in \mathscr{G}(n; k)\}$, $\varrho_{min}(\mathscr{G}; n, k) = \min\{\varrho(G) \mid G \in \mathscr{G}(n; k)\}$, $\varrho_{max}(\mathscr{T}; n, k) = \max\{\varrho(T) \mid T \in \mathscr{T}(n; k)\}$, $\varrho_{min}(\mathscr{T}; n, k) = \min\{\varrho(T) \mid T \in \mathscr{T}(n; k)\}$.

Let u, v be two vertices of a connected graph G. Suppose $v_1, v_2, \ldots, v_s (1 \le s \le deg(v))$ are some vertices of $N_G(v) \setminus N_G[u] (N_G[u] = N_G(u) \bigcup \{u\})$. Let G^* be the graph obtained from G by deleting the edges (v, v_i) and adding the edges $(u, v_i) (1 \le i \le s)$ (see Fig. 1.1). We call the process from G to G^* a *graft transformation*. An interesting thing is that a *graft transformation* always changes the distance spectral radius (adjacency spectral radius [10], signless Laplacian spectral radius [11]) of a graph. In this paper, some graft transformations that decrease or increase $\varrho(G)$ are presented. With them, for the graphs with both order n and k pendant vertices, the extremal graphs with the minimum distance spectral radius are completely characterized; the extremal graph with the maximum distance spectral radius is shown to be a dumbbell graph when $2 \le k \le n-2$; for $k = 1, 2, 3, n-1$, the extremal graphs with the maximum distance spectral radius are completely characterized respectively.

2. Graft transformations

Lemma 2.1 ([12]). *Let A be an $n \times n$ real symmetric irreducible nonnegative matrix and $X \in R^n$ be an unit vector. If $\rho(A) = X^T AX$, then $AX = \rho(A)X$.*

Definition 2.2. The union of simple graphs H and G is the simple graph $G \bigcup H$ with vertex set $V(G) \bigcup V(H)$ and edge set $E(G) \bigcup E(H)$. The intersection $G \bigcap H$ of simple graphs H and G is defined analogously.

Theorem 2.3. *Suppose graph $G = \bigcup_{i=1}^{3} G_i$ satisfies that $G_i \bigcap G_j = v_0$ for $1 \le i, j \le 3, i \ne j$, and that $|V(G_i)| \ge 2$ for $i = 1, 2, 3$ (see Fig. 2.1). $X = (x_0, x_1, \ldots, x_{n-1})^T$ is the Perron eigenvector corresponding to $\varrho(G)$, in which x_i corresponds to v_i. Let $S_1 = \sum_{v_i \in V(G_1)} x_i$, $S_2 = \sum_{v_i \in V(G_2)} x_i$, and for a vertex $v_a \in V(G_2)$, $v_a \ne v_0$, let graph $H = G - \sum_{v_i \in N_{G_3}(v_0)} v_0 v_i + \sum_{v_i \in N_{G_3}(v_0)} v_a v_i$. If $S_1 \ge S_2$, then $\varrho(H) > \varrho(G)$.*

Proof. Suppose that $P_{a,0}$ is a shortest path from v_a to v_0 in G_2 with length $d_a \ge 1$. Note that for $v_i \in V(G_3) \setminus \{v_0\}$, $v_j \in V(G_1)$, we have $d_H(v_i, v_j) - d_G(v_i, v_j) = d_a$; for $v_i \in V(G_3) \setminus \{v_0\}$, $v_k \in V(G_2)$, we have $d_G(v_i, v_k) - d_H(v_i, v_k) \le d_a$. So

$$\varrho(H) - \varrho(G) \ge X^T D(H)X - X^T D(G)X \ge 2d_a(S_1 - S_2) \sum_{v_i \in V(G_3) \setminus \{v_0\}} x_i \ge 0.$$

Suppose $\varrho(H) = \varrho(G)$, then $X^T D(H)X = \varrho(H)$. By Lemma 2.1, $D(H)X = \varrho(H)X$, but $\varrho(H)x_0 = D(H)_0 X > D(G)_0 X = \varrho(G)x_0$, where $D(H)_0$, $D(G)_0$ denote the rows corresponding to v_0 in $D(H)$, $D(G)$ respectively. So, $\varrho(H) \ne \varrho(G)$ and then $\varrho(H) > \varrho(G)$. $\square$

Same as proof of Theorem 2.3, we can prove the following theorem.

Theorem 2.4. *Graph G as shown in Fig. 2.2 satisfies that $G_1 \bigcap G_3 = v_1$, $v_1 v_2$ is a cut edge. $X = (x_1, x_2, \ldots, x_n)^T$ is the Perron eigenvector corresponding to $\varrho(G)$, in which x_i corresponds to v_i. Let $S_1 = \sum_{v_i \in V(G_1)} x_i$, $S_2 = \sum_{v_i \in V(G_2)} x_i$, and let graph $H = G - \sum_{v_i \in N_{G_3}(v_1)} v_1 v_i + \sum_{v_i \in N_{G_3}(v_1)} v_2 v_i$. If $S_1 \ge S_2$, $|V(G_3)| \ge 2$, then $\varrho(H) > \varrho(G)$.*

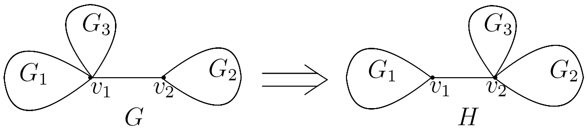

Fig. 2.2. G, H.

Fig. 3.1. G.

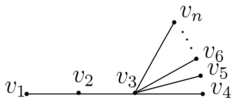

Fig. 3.2. H.

3. Extremal graphs

For a nonnegative irreducible square matrix A, the *spectralradius*, denoted by $\rho(A)$, is the maximum of the moduli of its eigenvalues.

Lemma 3.1 ([13]). *Suppose both A, B are nonnegative irreducible and $B \leq A$ (namely $B_{i,j} \leq A_{i,j}$ for each pair of i, j). Then $\rho(B) \leq \rho(A)$ with equality if and only if $B = A$.*

Lemma 3.2 ([14]). *Suppose that G_1 is a complete graph with $V(G_1) = \{v_0, v_{k+1}, v_{k+2}, \ldots, v_{n-1}\}$ $(n - 3 \geq k)$. Graph G consists of the complete graph G_1 and pendant edges $v_0v_1, v_0v_2, \ldots, v_0v_k$. Graph H consists of G_1 and pendant stars S_{t_i} attached at each vertex v_i (v_i is the center of S_{t_i}) of the complete graph G_1 where stars can be trivial (with only one vertex). Then we have*

(i) *if $k = 0, 1$, then $\varrho(H) = \varrho(G)$;*
(ii) *if $k \geq 2$ and $2 \leq t_0 < k + 1$, then $\varrho(H) > \varrho(G)$.*

Theorem 3.3. *If graph $G \in \mathscr{G}(n; k)$ satisfies that $\varrho(G) = \varrho_{min}(\mathscr{G}; n, k)$, then*

(i) *for $n = 2$, $G \cong K_2$;*
(ii) *for $n \geq 1$, $n \neq 2$, $0 \leq k \leq n - 1$, $k \neq n - 2$, G is isomorphic to a graph obtained by attaching k pendant edges to a vertex of a complete graph with order $n - k$;*
(iii) *for $n \geq 4$, $k = n - 2$, $G \cong D(n; 1, n - 3)$.*

Proof. (i) clearly holds.

(ii) clearly holds for $k = n-1$. Next we consider the case that $k \leq n-3$. Suppose that $v_1, v_2, \ldots, v_{n-k}$ are the non-pendant vertices of G. By Lemma 3.1, we know that for a connected graph $\mathscr{D}$, if $uv \notin E(\mathscr{D})$ $(u, v \in V(\mathscr{D}))$, then $\varrho(\mathscr{D} + uv) < \varrho(\mathscr{D})$. Therefore, in G, if $G[v_1, v_2, \ldots, v_{n-k}]$ is not a clique (complete subgraph), by adding edges to $G[v_1, v_2, \ldots, v_{n-k}]$, we can get a new graph H satisfying that $H[v_1, v_2, \ldots, v_{n-k}]$ is a clique. Then $\varrho(H) < \varrho(G)$, which contradicts $\varrho(G) = \varrho_{min}(\mathscr{G}; n, k)$. So $G[v_1, v_2, \ldots, v_{n-k}]$ must be a clique. Then for $k \leq n - 3$, (ii) follows from Lemma 3.2.

It is easy to check that (iii) holds for $n = 4, 5$ (see Fig. 3.1). Next we suppose $n \geq 6$. $H \cong D(n; 1, n - 3)$ is as shown in Fig. 3.2. $X = (x_1, x_2, \ldots, x_n)^T$ is the Perron eigenvector corresponding to $\varrho(H)$, in which x_i corresponds to v_i.

By symmetry, $x_4 = x_5 = \cdots = x_n$. Let $M = \sum_{i=3}^{n} x_i$. Note that $\varrho(H)x_1 - \varrho(H)x_2 = M + x_2 - x_1$. Then $(\varrho(H) + 1)(x_1 - x_2) = M$. So we have $x_1 > x_2$. Note that $\varrho(H)x_1 - \varrho(H)x_4 = (n - 1)x_4 + x_3 - x_2 - 3x_1$. So $(\varrho(H) + n - 1)(x_1 - x_4) = (n - 4)x_1 + x_3 - x_2$. Then we have $x_1 > x_4$. Note that $\varrho(H)(x_3 + x_4 + x_5) - \varrho(H)(x_1 + x_2) = 4x_2 + 7x_1 - 4x_4 - x_3$. So we have $(\varrho(H) + 1)(x_3 + x_4 + x_5 - (x_1 + x_2)) = 3x_2 + 6x_1 - 2x_4 > 0$. Then $x_3 + x_4 + x_5 > x_1 + x_2$, and so $x_3 + x_{n-1} + x_n > x_1 + x_2$. For $4 \leq j \leq n - 1$, we let $H' = H - \sum_{i=4}^{j} v_3v_i + \sum_{i=4}^{j} v_2v_i$. When $j = n - 1$, Then $H' \cong H$. When $4 \leq j \leq n - 2$, by Lemma 2.4, we get $\varrho(H') > \varrho(H)$. With these, we get that for $k = n - 2$, if $\varrho(G) = \varrho_{min}(\mathscr{G}; n, k)$, then $G \cong H$. Then (iii) follows. □

Theorem 3.4. *Suppose that graph $G \in \mathscr{T}(n; k)$ and $\varrho(G) = \varrho_{max}(\mathscr{T}; n, k)$ $(2 \leq k \leq n - 2)$. Then $G \in \mathscr{D}(n, k; s, p)$.*

Proof. Assume that the theorem does not hold. Suppose that $P_d = P_1 \bigcup P_2$ is a diameter-path of G, where path $P_1 = v_sv_{s-1} \ldots v_1v_0$, $P_2 = v_0v_{s+1}v_{s+2} \ldots v_d$. Suppose $G = \bigcup_{i=1}^{3} T_i$, where $T_i \bigcap T_j = v_0$ for $j \neq i$, $1 \leq i, j \leq 3$, and $P_1 \subseteq T_1$, $P_2 \subseteq T_2$. If $d(T_3) \geq 2$, then both the lengths of P_1 and P_2 are at least 2. Suppose that $X = (x_0, x_1, \ldots, x_{n-1})^T$ is the Perron eigenvector corresponding to $\varrho(G)$, in which x_i corresponds to v_i. Let $S_1 = \sum_{v_i \in V(T_1)} x_i$, $S_2 = \sum_{v_i \in V(T_2)} x_i$. Suppose $S_1 \geq S_2$. Let $H = G - \sum_{v_i \in N_{T_3}(v_0)} v_0v_i + \sum_{v_i \in N_{T_3}(v_0)} v_{d-1}v_i$. Then $\varrho(H) > \varrho(G)$ by Theorem 2.3 and $d(H) \geq d(G) + 1$. Proceeding like this, we get a caterpillar graph $\mathscr{H}$ with diameter $n - k + 1$ (see Fig. 3.3).

Suppose that $P = v_{a(1,1)}v_1v_2 \ldots v_{n-k-1}v_{n-k}v_{a(n-k,1)}$ is a diameter-path in $\mathscr{H}$. Denote by $v_iv_{a(i,j)}$ $(0 \leq j \leq t_i)$ the pendant edges attaching to vertex v_i $(1 \leq i \leq n - k)$. If there exists $t_b > 0$, $2 \leq b \leq n - k - 1$, let $\mathbb{S}_b = \bigcup_{j=1}^{t_b} v_bv_{a(b,j)}$. Suppose that

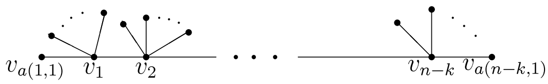

Fig. 3.3. $\mathscr{H}$.

$\mathscr{H} = T_1' \bigcup T_2' \bigcup \mathbb{S}_b, T_1' \bigcap T_2' = T_1' \bigcap \mathbb{S}_b = T_2' \bigcap \mathbb{S}_b = v_b, v_1 \in V(T_1'), v_{n-k} \in V(T_2')$. Suppose that $Y = (y_0, y_1, \ldots, y_{n-1})^T$ is the Perron eigenvector corresponding to $\varrho(\mathscr{H})$, in which y_i corresponds to v_i. Let $S_1' = \sum_{v_i \in V(T_1')} y_i, S_2' = \sum_{v_i \in V(T_2')} y_i$. Suppose $S_1' \geq S_2'$. Let $\mathscr{H}_1 = \mathscr{H} - \sum_{j=1}^{t_b} v_b v_{a(b,j)} + \sum_{j=1}^{t_b} v_{n-k} v_{a(b,j)}$. Then $\varrho(\mathscr{H}_1) > \varrho(\mathscr{H})$ by Theorem 2.3. Proceeding like this, we get a graph $\mathscr{H} \in \mathscr{D}(n, k; s, p)$ such that $\varrho(\mathscr{H}) > \varrho(\mathscr{H}_1)$, which contradicts $\varrho(G) = \varrho_{max}(\mathscr{T}; n, k)$. Therefore, the theorem holds. □

Lemma 3.5 ([15]). *Denote by $G(v, k)$ the graph obtained from a graph G by attaching a pendant path $P = v_0v_1v_2 \ldots v_k$ to a vertex $v = v_0$ of G, and denote by ϱ the distance spectral radius of $G(v,k)$. Let $X = (x_0, x_1, \ldots, x_{n-1})^T$ be the Perron vector corresponding to ϱ, in which x_i corresponds to v_i, and let $S = \sum_{i=0}^{n-1} x_i$. Then $\sum_{i=1}^{k} x_i = x_0 f(k) + \frac{S}{\varrho} g(k)$, where $\varrho = \varrho(G(v, k))$, $f(x) = \frac{t(t^{2x}-1)}{(1+t^{2x+1})(t-1)}$ and $g(x) = \frac{t(t^x-1)(t^{x+1}-1)}{(1+t^{2x+1})(t-1)^2}$ with $t = 1 + \frac{1}{\varrho} + \frac{\sqrt{2\varrho+1}}{\varrho}$. Furthermore, the functions $f(x)$ and $g(x)$ are monotonically increasing.*

Lemma 3.6 ([16]). *Let w be a vertex of a nontrivial connected graph G and for nonnegative integers p and q, and let $G(p, q)$ denote the graph obtained from G by attaching pendant paths $P = wv_1v_2 \ldots v_p$ and $Q = wu_1u_2 \ldots u_q$. If $p \geq q \geq 1$, then $\varrho(G(p, q)) < \varrho(G(p + 1, q - 1))$.*

Theorem 3.7. *If graph $G \in \mathscr{G}(n; k)$ with $2 \leq k \leq n - 2$ and $\varrho(G) = \varrho_{max}(\mathscr{G}; n, k)$, then*

(i) *$G \in \mathscr{D}(n, k; s, p)$.*

(ii) *Suppose that G is obtained by attaching pendant edges $v_1v_{n-k+1}, v_1v_{n-k+2}, \ldots, v_1v_{n-k+s}$ to vertex v_1 of a path $P = v_1v_2 \ldots v_{n-k-1}v_{n-k}$ and attaching pendant edges $v_{n-k}v_{n-k+s+1}, v_{n-k}v_{n-k+s+2}, \ldots, v_{n-k}v_n$ to vertex v_{n-k}. $X = (x_1, x_2, \ldots, x_n)^T$ is the Perron eigenvector corresponding to $\varrho(G)$, in which x_i corresponds to v_i. Let $S_1 = \sum_{i=n-k+1}^{n-k+s} x_i, S_2 = \sum_{n-k+s+1}^{n} x_i$. If $s \geq p$, then $S_1 \geq S_2$, but $x_{n-k+1} \leq x_{n-k+s+1}$. In particular, $x_{n-k+1} < x_{n-k+s+1}$ if $s > p$.*

Proof. (i) By Theorem 3.4, we may assume that G is not a tree. Suppose that H is a spanning tree of G. By Lemma 3.1, we know that for a simple connected graph $\mathscr{B}$, if $uv \in E(\mathscr{B})$ and $\mathscr{B} - uv$ is also connected, then $\varrho(\mathscr{B} - uv) > \varrho(\mathscr{B})$. So, $\varrho(H) > \varrho(G)$. Suppose $\mathcal{K}(H) = \varepsilon$, then $\varepsilon \geq k$. By Theorem 3.4, we can get a graph $H_1 \in \mathscr{D}(n, \varepsilon; r, t)$ such that $\varrho(H_1) \geq \varrho(H)$. Suppose H_1 is obtained by attaching r pendant edges to the vertex v_1 of a path $P' = v_1v_2 \ldots v_{n-\varepsilon}$ and attaching t pendant edges to the vertex $v_{n-\varepsilon}$.

If $\max\{r, t\} \geq k$, for convenience, we suppose $\max\{r, t\} = r$. Using Lemma 3.6 repeatedly, we can get a graph H_2 that $\varrho(H_2) > \varrho(H_1)$ from H_1 by deleting $r - k + 2$ pendant edges attaching at vertex v_1 and deleting all the pendant edges attaching at vertex $v_{n-\varepsilon}$, and then attaching a pendant path with length $r - k + 2$ to vertex v_1 and attaching a pendant path with length t to vertex $v_{n-\varepsilon}$.

If $\max\{r, t\} < k$, for convenience, we suppose $\max\{r, t\} = r$. Using Lemma 3.6 repeatedly, we can get a graph H_2 that $\varrho(H_2) > \varrho(H_1)$ from H_1 by deleting $\varepsilon - k + 1$ pendant edges attaching at vertex $v_{n-\varepsilon}$, and then attaching a pendant path with length $\varepsilon - k + 1$ to vertex $v_{n-\varepsilon}$.

For both above two cases, $\mathcal{K}(H_2) = k$. By Theorem 3.4, we can get a graph $\mathscr{H} \in \mathscr{D}(n, k; s, p)$ such that $\varrho(\mathscr{H}) > \varrho(H_2)$, which contradicts $\varrho(G) = \varrho_{max}(\mathscr{G}; n, k)$. Therefore, (i) holds.

(ii) Suppose $s \geq p$. By symmetry, $x_{n-k+1} = x_{n-k+2} = \cdots = x_{n-k+s}, x_{n-k+s+1} = x_{n-k+s+2} = \cdots = x_n$. Assume that $S_2 > S_1$, then $x_{n-k+1} < x_{n-k+s+1}$. By Lemma 3.5, we get $x_1 < x_{n-k}$.

1° $n - k$ is odd. Note that, for $1 \leq i \leq \lfloor \frac{n-k}{2} \rfloor - 1$,

$$\varrho(G)(x_{n-k-i} - x_{i+1}) - \varrho(G)(x_{n-k-i+1} - x_i) = 2\left(\sum_{j=n-k-i+1}^{n-k} x_j + S_2\right) - 2\left(\sum_{j=1}^{i} x_j + S_1\right) > 0.$$

Because $x_1 < x_{n-k}$, by induction, we can get $x_{n-k-i} - x_{1+i} > 0$ for $0 \leq i \leq \lfloor \frac{n-k}{2} \rfloor - 1$. But

$$\varrho(G)\left(x_{\frac{n-k+3}{2}} - x_{\frac{n-k-1}{2}}\right) = 2\left(\sum_{j=1}^{\frac{n-k-1}{2}} x_j + S_1\right) - 2\left(\sum_{j=\frac{n-k+3}{2}}^{n-k} x_j + S_2\right)$$

$$\Rightarrow (\varrho(G) + 2)\left(x_{\frac{n-k+3}{2}} - x_{\frac{n-k-1}{2}}\right) = 2\left(\sum_{j=1}^{\frac{n-k-3}{2}} x_j + S_1\right) - 2\left(\sum_{\frac{n-k+5}{2}}^{n-k} x_j + S_2\right) < 0,$$

which contradicts that $x_{n-k-i} - x_{1+i} > 0$ for $0 \leq i \leq \lfloor \frac{n-k}{2} \rfloor - 1$.

2° $n-k$ is even. As 1°, we can get the same contradiction.

From 1° and 2°, we get $S_1 \geq S_2$. Assume that $x_{n-k+1} \geq x_{n-k+s+1}$ if $s > p$, we can get the same contradictions as 1° and 2°. Therefore, (ii) holds. □

Lemma 3.8 ([14]). *Let G be a connected unicyclic graph with order n ($m(G) = n$, $n \geq 3$). Then $\varrho(G) \leq \varrho(P_n')$ where P_n' is obtained from a triangle K_3 by attaching pendent path with length $n-3$ to one of its vertices, with equality if and only if $G \cong P_n'$.*

Theorem 3.9. *If graph $G \in \mathscr{G}(n; k)$ with n and $\varrho(G) = \varrho_{\max}(\mathscr{G}; n, k)$, then*

(1) *for $n = 1$, we have $k = 0$ and $G \cong K_1$;*
(2) *for $n = 2$, we have $k = 2$ and $G \cong K_2$;*
(3) *for $n = 3$, we have $k = 0$ and $G \cong K_3$, or we have $k = 2$ and $G \cong P_3$;*
(4) *for $n \geq 3$, $k = n-1$, we have $G \cong S_n$;*
(5) *for $n \geq 4$, $k = 1$, we have $G \cong P_n'$ where P_n' is as in Lemma 3.8;*
(6) *for $n \geq 4$, $k = 2$, we have $G \cong P_n$;*
(7) *for $n \geq 5$, $k = 3$, we have $G \cong D(n; 1, 2)$.*

Proof. (1), (2), (3), (4) are obvious. (6), (7) follows from Theorem 3.7.

For a graph $H \in \mathscr{G}(n; 1)$, H is not a tree. Thus H contains cycles. If H is not a unicyclic graph. By delete some edges of H, we can get a connected unicyclic graph $\mathscr{B}$. By Lemma 3.1, then $\varrho(\mathscr{B}) > \varrho(H)$. By Lemma 3.8, we know that $\varrho(P_n') \leq \varrho(\mathscr{B})$, with equality if and only if $\mathscr{D} \cong P_n'$. Note that there is only one pendant vertex in P_n'. Then (5) follows. □

4. Conjecture

Based on computational evidence, we make the following conjecture.

Conjecture 4.1. *If graph $G \in \mathscr{G}(n; k)$ ($4 \leq k \leq n-2$) satisfying $\varrho(G) = \varrho_{max}(\mathscr{G}; n, k)$, then $G \cong D(n; \lceil \frac{k}{2} \rceil, \lfloor \frac{k}{2} \rfloor)$.*

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